

Searching for Topological Degeneracy in the Hubbard Model with Quantum Monte Carlo

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Z_2 spin liquids have topological order. One manifestation of this is that a Z_2 spin liquid on a torus exhibits a four-fold degeneracy. Recent numerical evidence has argued for the existence of a spin liquid ground state in the Hubbard model on a honeycomb lattice near $U \approx 4$ [10]. The evidence for this claim involves the presence of a gapped state that lacks any identifiable order. This argument relies on being able to distinguish small order from no order which is notoriously difficult. In this paper we demonstrate an approach which uses quantum Monte Carlo to search for one of the key features that positively identify the topological spin liquid: the topological degeneracy. For any finite system, this topological degeneracy is split where the splitting decays exponentially with system size. We search for low lying states in the energy spectrum that could be identified as these topologically degenerate states. We show that, for system sizes up to $N = 162$ sites, there is no evidence for these states being significantly below the first excited state giving evidence against the existence of a topological phase. We discuss the possible options for the Hubbard model on the honeycomb lattice in the absence of such degeneracy.

Introduction Most physical systems are either gapless or order at low temperatures, spontaneously breaking a symmetry. Systems which fail to do so are usually exotic and often demonstrate interesting properties such as topological order. In fact, a famous theorem of Hastings [6] states that systems with an odd number of sites per unit cell and no broken symmetries must either be gapless or topologically ordered. One manifestation of this topological order is that the system has a ground state degeneracy which depends on the topological manifold on which the system lives. Recent work [10] has given strong numerical evidence that the Hubbard model on the honeycomb lattice at intermediate U ($3.5 \lesssim U \lesssim 4.25$) is gapped (both in the spin and charge sectors) and has no order/broken symmetries. As Z_2 spin liquids are gapped and typically have no broken symmetries, this numerical result has been taken as evidence for a spin-liquid ground state on the Hubbard honeycomb model. Z_2 spin liquids also have topological order [2, 8, 13]. Because the honeycomb lattice has two sites per unit cell, Hasting's theorem is not directly applicable. This leaves open a key question: is the system actually topological?

Either a positive or negative answer to this question is intrinsically interesting. Finding topological order would give the first positive indication of the Z_2 spin liquid state and supply the key missing piece of evidence in making the case for this phase. To date, all evidence for the spin liquid has involved the heroic task of ruling out all other possible ordered states. This requires extrapolating many order parameters to the thermodynamic limit and distinguishing a small value from zero. We propose that searching for the ground state degeneracy may be a more robust qualitative feature that doesn't require distinguishing small differences.

On the other hand, finding no ground state degeneracy would rule out the interpretation of the numerical results given in ref. [10]. This then would leave three alternative

possibilities: (1) There is some order in the system. (2) The system is actually gapless. (3) The ground state is a gapped phase with no broken symmetries and is not topological. This latter possibility must be a Mott insulator as band insulators that don't break symmetries are forbidden on the honeycomb lattice at half filling [7]. This would be particularly intriguing as even this Mott insulating case is forbidden when there are an odd number of sites per unit cell. Although featureless insulators have been discussed in ref. [7], no simple local fermionic Hamiltonian which supports (3) as a potential ground state are currently known. In addition, finding such an example would further emphasize the importance of establishing the topological nature as a necessary step in identifying spin liquids.

In this work, we compute properties of the low-lying spectrum of the Hubbard model on the honeycomb lattice with the motivation of looking for "degenerate" ground states. We accomplish this by developing an approach which combines quantum Monte Carlo calculations with analytical bounds on how high-energy states can influence the low temperature entropy. In the process, we develop evidence against the presence of topological degeneracy. We do this by showing that, for finite-size systems, the low-lying spectrum of the ground state does not include any states that can be identified as the "degenerate" ground states. Unfortunately, we can not definitively conclude whether this is because the topological degeneracy for this system is absent or the system sizes we can simulate are too small to see the "topologically degenerate" states. In particular, the correlation length may be such that those states lie above the first excited state for the simulated system sizes.

Background In this work, we are interested in the

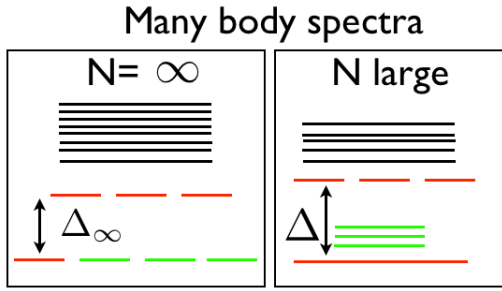


Figure 1: Cartoon representation of the expected spectra for the Z_2 spin liquid on the Hubbard honeycomb model for $N = \infty$ and large N . At $N = \infty$ (on a torus), there are four degenerate ground states and then a gap to the (in this case) three degenerate excited states. The four degenerate ground states (shown in green) split at finite N due to finite size effects; we label them TDGS. The finite size-ground state and three excited states (shown in red) have a (finite-size) gap identified by ref [10]; these four states are labelled as the reference spectrum and used as a baseline to compare against spectra which include TDGS. Other excited states lie above the first excited state, but such states can only increase the entropy $S(\beta)$.

Hubbard model on a honeycomb lattice given by

$$H = -t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i (n_{i\uparrow} + 1/2)(n_{i\downarrow} - 1/2) + \mu \quad (1)$$

where σ denotes spin \uparrow, \downarrow , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ and we set the chemical potential $\mu = 0$ so the system is at half filling. Interest in this system was stimulated by numerical evidence [10] for a spin liquid. Since this time, a number of concrete spin liquid states have been proposed [5, 9, 12, 14]. These states are primarily Z_2 spin liquids and therefore have (on a torus) four degenerate ground states. The latter spin liquid proposal [14] involves additional symmetries and requires a 16-fold degeneracy. Our primary focus in this paper will be searching for four degenerate ground states.

In any finite system, the degeneracy of these states will be broken leaving a single “finite-size ground state” and three additional “finite-size excited states” in the spectrum (see fig. 1). In the limit of large N , these states will approach the true ground state exponentially quickly. Therefore evidence for topological degeneracy could be found by looking for three excited states in the low-lying spectrum that are not identifiable as other excitations (i.e. spin/charge excitations) and ideally fall (significantly) below the true first excited state. We denote these extra three states as thermodynamically degenerate ground states (TDGS). The true thermodynamic first excited state is identified by ref. [10] as coming from the staggered spin sector and therefore is presumably a three-fold degenerate spin triplet (this fact is also consistent with our results). We notate the ground state and three true first excited states as the reference spectrum. It is the existence of states (significantly) below this in which

we are therefore most interested. In this work, for finite size systems, we (a) examine whether the available data can be accurately fit without resorting to the existence of additional eigenstates in addition to the reference spectrum (such as the TDGS) and (b) place bounds on how low the TDGS can be in the many-body spectrum. Our focus will be at $U = 4$ where the system appears to have no broken symmetries.

The methodology we use in this work is a finite temperature version of Determinant Quantum Monte Carlo (FTDQMC) [3]. Using FTDQMC we can compute properties of eqn. (1) at finite temperature which is naturally sensitive to all excitations independent of their origin. This is to be contrasted to the approach used in ref. [10] which is a projection technique. This latter technique is designed to project down to the true finite size ground state and, although sensitive to the gap, this sensitivity strongly depends on the overlap of the finite-size excited states with the initial trial state Ψ_T . This means the TDGS might be (for all practical purposes) invisible to this ground state method.

Entropy One place where a ground state degeneracy should be manifest is in the entropy at large inverse temperature $\beta \equiv 1/k_B T$. In particular, in the thermodynamic limit, a degenerate system will have a ground state entropy of the logarithm of the degeneracy. In a finite system, although this degeneracy breaks, one might expect to see instead plateaus at large β . One nice feature of the entropy is that it is a completely unbiased way to search for the presence of excitations as it is sensitive only to their energy eigenvalues placing no constraints on accurately identifying their quantum numbers, etc.

There are many approaches for computing the entropy of a physical system. In this paper, we compute the entropy from many body spectra as well as from the functional dependence of the energy $U(\beta)$ on the inverse temperature β .

Given a set of eigenvalues E_i corresponding to a many body spectra, the entropy of the system at a given β is

$$S(\beta) = - \sum_i p_i(\beta) \ln p_i(\beta) \quad (2)$$

where p_i is the probability of the eigenstate i ,

$$p_i(\beta) = \frac{\exp(-\beta E_i)}{\sum_i \exp(-\beta E_i)} \quad (3)$$

On the other hand the temperature dependence of $U(\beta)$ can be used to compute the entropy via thermodynamic integration as

$$S(\beta) = S(0) - \left[\int_0^\beta U d\beta - \beta U(\beta) \right] \quad (4)$$

As our simulations are run in the grand canonical ensemble, we always have that $S(0) = 4^N$ where N is the total number of sites in our system.

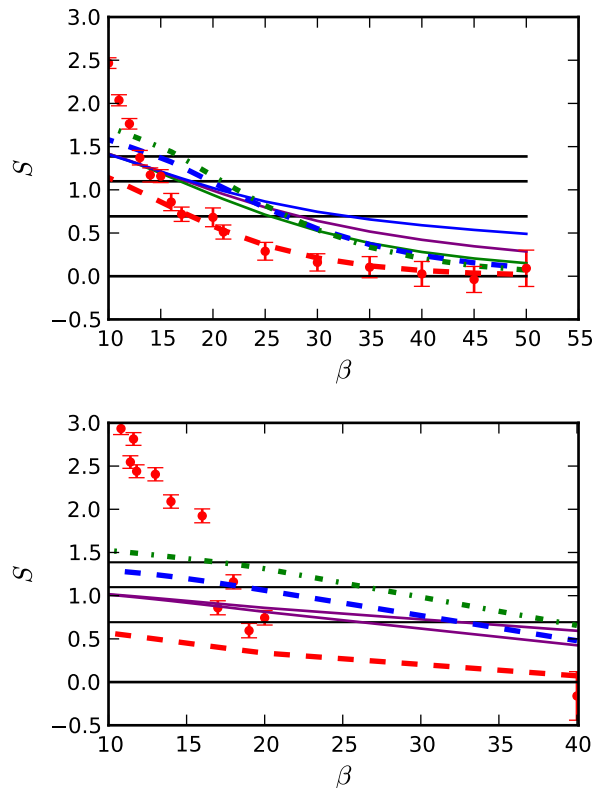


Figure 2: Entropy (red dots) for $N = 72$ at $\tau = 0.01$ (top) and $N = 162$ at $\tau \rightarrow 0$ (bottom). Time step errors and discretization errors have been checked to be negligible. The red dotted line shows the entropy of the reference spectrum using Δ from [10]. All other curved lines assume this spectrum plus additional states. Curved solid lines (from top to bottom) include an additional TDGS at (0.03, 0.05, 0.07) (top) and (0.03, 0.05) (bottom) respectively. The dashed blue line is the manifold of lowest entropies for having two TDGS below 0.1 (top) or 0.07 (bottom). The dot-dashed green line is the manifold of lowest entropies for having three TDGS below 0.12 (top) or 0.07 (bottom). Black lines are visual guides to the eye at 0, $\ln 2$, $\ln 3$, $\ln 4$.

For each β (on a fine grid) we compute the energy of the system. This energy can then be converted to an entropy using eqn. 4 and seen in fig. 2 for $N = 72, 162$. Notice that the entropy does not plateau at $\log 4$ (or $\log 3$ or $\log 2$) as would be expected if three (or two or one respectively) TDGS lie significantly below the finite-size first excited state. We additionally plot the entropy for the reference spectrum using the gap Δ found in ref. [10] assuming a triply degenerate excited state. We find that this curve favorably fits the entropy at large β giving no indication of the need for additional low lying eigenstates. Of course, a priori, it is not implausible that a series of additional excitations above and below the first excited state conspire to produce a similar entropy at large β . To better quantify against this possibility, we make use of the following fact (see supplemental information): Fix the lowest k excited states of a many-

body spectrum. Any additional higher-energy excited states can only make the entropy $S(\beta)$ increase for all β . We proceed then to propose possible low energy spectra, compute $S(\beta)$ associated with these spectra and show that this entropy curve lies above the simulation data. As additional high energy excited states can only increase the entropy, this shows the data is inconsistent with the proposed low energy spectra. We focus on low-energy spectra involving states in the reference spectrum with the addition of 1-3 excitations below the true excited states. Fig. 2 (top) shows the entropy curves for a series of low-energy spectra for $N = 72$ that has a single additional TDGS at energies ranging from half the first excited state to 0.1 as well as the lowest entropy manifold for two states below 0.1 and three states below 0.12. Simulations for $N = 162$ are also shown. Notice the entropy of the proposed spectra all lie above the data ruling out the possibility of a state at these energies.

Energy A complementary approach to finding the eigenvalues of the low-lying spectra is to fit it to the internal energy $U(\beta)$ at large β . In particular, we take the reference spectrum and compute $U(\beta) = 1/Z \sum_i E_i \exp[-\beta E_i]$ where $Z = \sum_i \exp[-\beta E_i]$. It should be noted that while the entropy calculation (through thermodynamic integration, eqn. 4) depends on the energies at small β ($\beta \lesssim 25$ for the $N = 72$), fitting $U(\beta)$ to a low-lying spectrum is sensitive to energies at large β ($\beta \gtrsim 25$) which is significantly below the gap. In fig. 3 we plot the energy corresponding to the reference spectrum for $N = 72, 162$ with the gap Δ found in ref. [10] assuming again a triply degenerate excited state. We see that for both system sizes, the data is fit without the need for additional low-energy states to be assumed.

The nature of topologically distinct ground states is that there aren't any local operators that convert one topological ground state to the other. One, then, might be concerned that a quantum Monte Carlo approach that samples space by applying the operator $\exp[-\tau H]$ (admittedly in an auxiliary field space) might lock itself into one topological sector, effectively becoming non-ergodic. We argue, that, although possible, there is evidence that this is not the case. At infinite temperature ($\beta = 0$), we know that there are 4^n states which correctly sets $S(0)$. In addition, even at high, but non-infinite temperatures we suspect that the thermal fluctuations are sufficient to 'see' the topological states anticipating that if the topological state is not sampled, it only happens at lower temperatures. Since the entropy at β depends only on energies at temperatures higher than β , it would require the state to be affecting the energies at temperatures higher than $\beta \approx 15 - 20$ to affect the conclusions of our study. Also, if the simulation is missing states (at any temperature) this affects the energies at that temperature and, by having an incorrect integrand, the entropy. The entropy would then generically not integrate down to zero; our results are zero within error bars and so any large deviation is inconsistent with the data. An additional check of consistency is that the high energy (i.e. entropy) data,

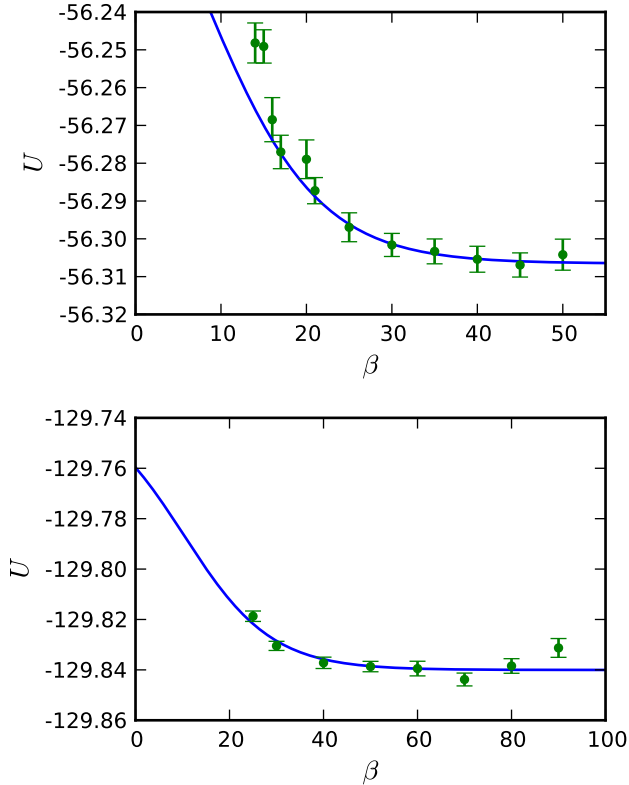


Figure 3: Energy of $N = 72$ (top) at $\tau = 0.01$ and $N = 162$ (bottom) at $\tau = 0.1$. The blue lines are $U(\beta)$ generated from the reference spectrum with a gap $\Delta = (0.1469226, 0.1071340)$ for $N = (72, 162)$ taken from ref. [10] with a single free parameter for the ground state energy selected to be $(-56.31, -129.84)$ respectively. There are no indications that additional energies are needed to fit U at large β .

the low energy data, and the spin gap measured by ref. [10] are all consistent with the same gap Δ ; moreover there is no obvious jump or non-monotonic behavior in the energies (which might be anticipated if some state disappeared for some temperatures). Finally, over many simulations, we have seen no evidence that the simulation sometimes finds one ground state and sometimes a “higher energy one” at low T as might be expected if it was randomly locking itself into one of many topological sectors. Although these considerations do not completely rule out the presence of non-ergodicity issues, we feel it makes it unlikely.

Discussion In this work, we have shown that, up to $N = 162$ sites, the evidence is strongly against the presence of states significantly below the spin triplet. Although the finite-size splitting between the TDGS are expected to decay exponentially with system size, there is the mundane possibility that at the system sizes at which we are able to perform calculations, the TDGS actually live high in the spectra and would come down for larger sizes. Although always impossible to rule out, the lack of any identifiable low lying states suggests alternative

explanations. We suggested three alternate possibilities in the introduction and find that there is supporting evidence in the literature for all three possibilities. Recent work [1, 11] has reconsidered the problem and reached a different conclusion than ref. [10] about the absence of magnetic order at $U \approx 4$ arguing for the existence of an ordered phase. Alternatively, ref. [4] considered a related model, the staggered-flux Hubbard model on a square lattice using an accurate (albeit approximate) method and found evidence for a gapless spin liquid. As the staggered-flux model can be continuously tuned to the honeycomb model by tuning the nearest neighbor hoppings, this can be taken as some evidence that a spin liquid phase on the honeycomb is more likely to be gapless than gapped; such a spin liquid would have no TDGS. Finally, there has been recent interest in both extending Hastings theorem to rule out featureless, non-topological states in other models as well as explicit examples where featureless states can exist [7]. Although none of these results currently speak directly to the honeycomb model, they do motivate the possibility that this is a featureless state which is consistent with the entirety of the results of [10].

Beyond giving evidence concerning the absence of the spin liquid phase on the Hubbard model, we have also demonstrated an approach which allows for identifying (or ruling out) the presence of degenerate ground states using quantum Monte Carlo. In particular, we use the entropy curve of model spectra as an effective way of showing that certain low-lying spectra are inconsistent with data irrespective of the continuum of excited states above them. Although not as accurate as exact diagonalization, this allows calculations on systems sizes (for sign-free problems) that go significantly beyond those that are reachable with a method which scales exponentially and we hope that these results encourage calculation of degenerate ground states in other putative spin liquid candidates.

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Supplemental information

In this appendix, we give a short proof that adding additional states in a spectrum above the largest energy E_{min} of a fixed low-energy reference spectrum can only increase the entropy.

Although there are many ways to show this fact, we use the following geometric argument. The entropy is defined as $S = -\sum_i p_i \ln p_i$. We can represent this

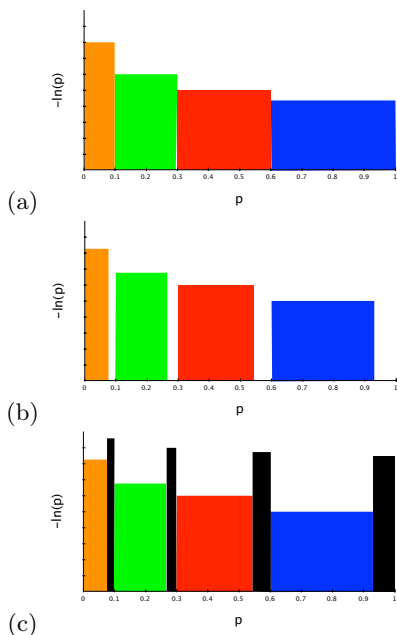


Figure 4: Area under the figures represent the entropy of a series of states: $-\sum_i p_i \ln p_i$. As more states are added which have smaller probability of being sampled, the area must increase.

geometrically as the area in a chart prototypically shown in fig. 4(a). Notice that we have $\sum_i p_i = 1$ where each $p_i = \exp[-\beta E_i]/Z$ with $Z = \sum_i \exp[-\beta E_i]$. When we add additional states the probability of the original states decreases as $p_i = \exp[-\beta E_i]/\tilde{Z}$ where $\tilde{Z} > Z$ as the sum is over more states. As $-\ln p$ monotonically increases as p gets smaller, the “height” taken by each of the former states in the reference spectrum strictly increases as see in fig. 4(b). By assumption, the added states are above all the original states in the reference spectrum (i.e. $E_{new} > E_{old}$) and therefore, for each j in the added states, $p_j = \exp[-\beta E_j]/\tilde{Z}$ must be smaller then each $p_i = \exp[-\beta E_i]/\tilde{Z}$ in the reference spectrum. Therefore, the “height” of each additional state must be larger then the height of any state in the reference spectrum as seen in fig. 4(c). Therefore, the total entropy (the area in the figure) must go up.

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- [1] Fakher F Assaad and Igor F Herbut. Pinning the order: the nature of quantum criticality in the hubbard model on honeycomb lattice. *arXiv preprint arXiv:1304.6340*, 2013.
 - [2] Leon Balents. Spin liquids in frustrated magnets. *Nature*, 464(7286):199–208, 2010.
 - [3] R. Blankenbecler, D.J. Scalapino, and R.L. Sugar. Monte carlo calculations of coupled boson-fermion systems. i. *Physical Review D*, 24(8):2278–2286, 1981.
 - [4] C.C. Chang and R.T. Scalettar. Quantum disordered phase near the mott transition in the staggered-flux hubbard model on a square lattice. *Physical Review Letters*, 109(2):26404, 2012.
 - [5] BK Clark, DA Abanin, and SL Sondhi. Nature of the spin liquid state of the hubbard model on honeycomb lattice. *arXiv preprint arXiv:1010.3011*, 2010.
 - [6] M. B. Hastings. Sufficient conditions for topological order in insulators. *EUROPHYS.LETT.*, 70:824, 2005. URL <http://www.citebase.org/abstract?id=oai:arXiv.org:cond-mat/0411094>.
 - [7] I. Kimchi, SA Parameswaran, A.M. Turner, and A. Vishwanath. Featureless and non-fractionalized bose insulator on the honeycomb lattice at 1/2 site-filling. *arXiv preprint arXiv:1207.0498*, 2012.
 - [8] Patrick A Lee. From high temperature superconductivity to quantum spin liquid: progress in strong correlation physics. *Reports on Progress in Physics*, 71(1):012501, 2008.
 - [9] Y.M. Lu and Y. Ran. Spin liquids on a honeycomb lattice: Projective symmetry group study of schwinger fermion mean-field theory. *arXiv preprint arXiv:1005.4229*, 2010.
 - [10] ZY MENG, TC LANG, S. WESSEL, FF ASSAAD, and A. MURAMATSU. Quantum spin liquid emerging in two-dimensional correlated dirac fermions. *Nature*, 464(7290):847–851, 2010.
 - [11] S. Sorella, Y. Otsuka, and S. Yunoki. Absence of a spin liquid phase in the hubbard model on the honeycomb lattice. *arXiv preprint arXiv:1207.1783*, 2012.
 - [12] F. Wang. Schwinger boson mean field theories of spin liquid states on a honeycomb lattice: Projective symmetry group analysis and critical field theory. *Physical Review B*, 82(2):024419, 2010.
 - [13] Xiao-Gang Wen. Quantum orders and symmetric spin liquids. *Physical Review B*, 65(16):165113, 2002.
 - [14] C. Xu. Quantum spin hall, triplet superconductor, and topological liquids on the honeycomb lattice. *Physical Review B*, 83(2):024408, 2011.